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Shoemaker wins graduate award



Daniel Shoemaker, a University of California, Santa Barbara (UCSB) graduate student and Lujan Neutron Scattering Center (LANSCE-LC) researcher, was awarded the Graduate Student Gold Award by the Materials Research Society (MRS) at the society's annual fall meeting. Shoemaker, a UCSB/Institute for Multiscale Materials Studies (IMMS) fellow, earned the award for his research in total scattering descriptions of local and cooperative Jahn-Teller distortions in the $\text{CuXMg}_{1-x}\text{Cr}_2\text{O}_4$ solid solution. He received a cash award and a presentation plaque.

Shoemaker has come to the Lujan Center since 2007, initially as a user and later as an IMMS fellow mentored by Anna Llobet and Thomas Proffen from the Total Scattering team in LANSCE-LC. His research, directed by Ram Seshadri (UCSB), uses neutron total scattering to describe structure-property relations in disordered, magnetic, and functional oxides. This includes least-squares refinement and reverse Monte Carlo simulations of the real-space pair distribution function. In the research for which he won the award, Shoemaker showed that Cu^{2+} forms significantly more distorted coordination environments than Mg^{2+} on the same crystallographic site, even in compounds that are a single crystalline phase as determined by Rietveld refinement. Local distortions remain prevalent in cases where long-range orbital ordering produces a cooperative Jahn-Teller distortion. He defended his thesis in September and began a postdoctoral appointment at Argonne National Laboratory.

The Materials Research Society is an organization of materials researchers from academia, industry, and government that promotes communication for the advancement of interdisciplinary materials research to improve the quality of life. MRS Graduate Student Awards are intended to honor and encourage graduate students whose academic achievements and current materials research display a high level of excellence and distinction. MRS seeks to recognize students of exceptional ability who show promise for significant future achievement in materials research. A panel of judges chose the graduate student award winners based on their oral presentations and application materials.

Page receives award at Los Alamos Postdoc Research Day

Katharine Page (LANSCE-LC) is the recipient of a poster award at the recent Los Alamos Postdoc Research Day for her work on "Probing Atomic Structure in Functional Thin Films and Nanoparticles." Her mentor is Thomas Proffen (LANSCE-LC).



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Colleagues,

As a national/international user facility, LANSCE's Web presence and communication with users are paramount. To that end, please join me in welcoming Elena Fernández as the LANSCE User Program Public Information Specialist. Elena is a communications professional, specialist, and alumna of New Mexico State University with a Bachelor of Arts in philosophy. She has worked in the various colleges and the departments of NMSU since 2003. Elena has held many functions in a variety of fields such as graphic artist, academic advisor, student recruiter, Web designer, and sub-contractor for Camp Dresser & McKee: Scientists and Engineers (environmental consultant). She has served on several committees at NMSU in student recruitment, student retention, and Engineering Physics program accreditation, to name a few. Elena has received four Awards of Excellence, 2007-2010, from the APEX Awards (2007-2010) for Publication Excellence, which are given annually for excellence in publications work by communications professionals around the globe and are based on excellence in graphic design, editorial content, and the ability to achieve overall communications effectiveness and excellence. All of her awards were for works articulating science and engineering to their respective communities, as well as academia and the general public. She is working diligently on LANSCE's Web presence. Even though, a lot of work is to be done you can now download the latest *Pulse*, the 2007-2009 LANSCE Activity Report in memory of Louis Rosen, and facilities proposal calls.



**Please join me
in welcoming
Elena Fernández
as the
LANSCE User
Program Public
Information
Specialist.**

Elena's office is in Building -1, Room B109, and her phone is 5-0541. Please stop by and welcome Elena.

Let me also take this opportunity and reiterate Kurt Schoenberg's message this past month related to the TA-53 Access Control Policy. This policy (TA53-PR-201-008.R5 on Mesalib) allows us to accommodate the needs of operating an international user facility. There are several important points that we all must follow in order to retain this site access flexibility.

Specifically:

- Foreign nationals must possess a Laboratory issued badge for access.
- Access by non-DOE badge holders, who are US Citizens, can be locally approved if they have official business on site or if they are part of an approved tour.
- Non-DOE badge holders, who routinely pick up or drop off TA-53 employees, can be granted access by obtaining a TA-53 Gate Access Pass from the Visitor Center with management concurrence. They explicitly cannot be granted access by having an administrator put them in the visitor database!
- Lab employees, who do not have their Lab-issued badge, must get a temporary badge from the LANL badge office. They cannot use the visitor access process to get on site.
- Access by non-DOE badge holders, for any other non-official-business reason, is not allowed.

LANSCE Deputy Division Leader Alex Lacerda



Page ... Many features [lattice, unique coordination or defects at the surface, ligand or capping groups, new (metastable) crystal structures, and shapes or architectures] give nanomaterials a distinct functionality compared with a bulk material of similar composition. Accurate determination of atomic structure is essential to understand and utilize resulting material properties and validate and aid computer models. Page advanced the atomic pair distribution function formalism of neutron and x-ray total scattering for the detailed atomic structure of functional thin films and nanoparticles. She demonstrated the contributions that these methods provide to study functional materials in the limits of size reduction.

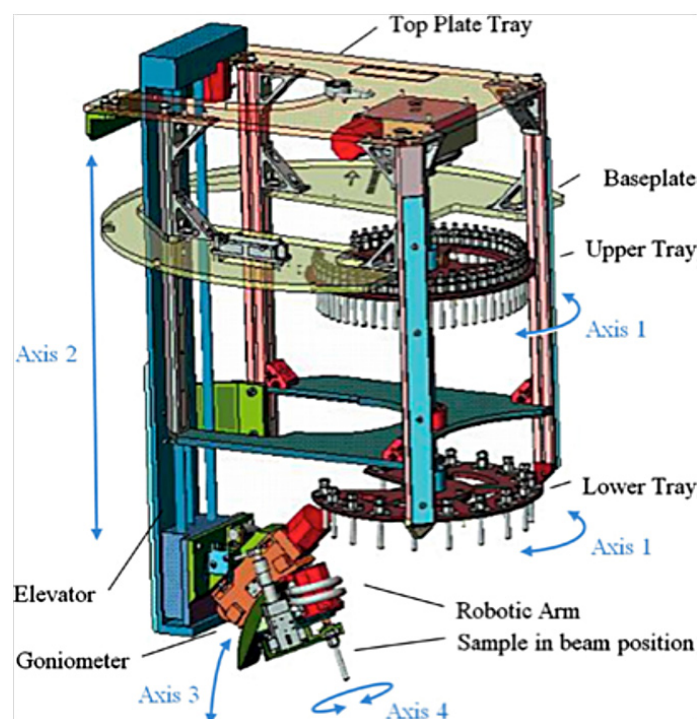
The Laboratory-wide Los Alamos Postdoc Research Day provided postdoctoral researchers the opportunity to present a summary of their Los Alamos research, receive feedback, and enhance collaboration and technical discussions among postdoctoral researchers and staff. The Los Alamos Postdoc Association and the Postdoc Program Office co-sponsored the event.

Versatile automated sample changer for texture measurements at LANSCE

In hosting neutron diffraction users at the LANSCE Lujan Neutron Scattering Center, efficiency is paramount. Short count times per sample on modern neutron diffractometers allow for high sample throughput. Automation of sample changes is essential to optimize the usage of available neutron flux and reduce the instrument downtime due to closing and opening of shutters and sample alignment.

Researchers installed an automated sample changer with an Eulerian cradle for neutron texture measurements in the high pressure-preferred orientation instrument (HIPPO). ZYGO/Square One Systems Design originally designed and manufactured the sample changer hardware, and LANSCE developed the control software. H. M. Reiche (New Mexico State University and LANSCE-LC) and S. C. Vogel (LANSCE-LC) developed and improved the system. All electronic devices (motion control, network switch, etc) are mounted on top of the sample changer. Only the power and network cable must be connected for operation, allowing setup of the sample changer in HIPPO within a few minutes. The device has successfully measured more than 2,300 texture and almost 400 powder samples at ambient conditions since it became operational. The automated sample changer significantly reduces the time required to change samples and allows unattended operation of the instrument. Its three degrees of freedom allow for versatile use for texture analysis and sample alignment. Combined with HIPPO sample environment capabilities, the fast sample turnaround is an

essential tool to investigate materials properties under extremes of temperature and pressure. Operating the device for almost a decade has resulted in sustained enhancements of mechanics, electronics and software, which significantly improved reliability and resiliency. By standardizing both the flange of the sample wells and the beam position relative to that flange, this sample changer, like many other sample environments at LANSCE, is portable and fits into four different diffractometers of LANSCE (HIPPO, neutron powder diffractometer, spectrometer for materials research at temperature and stress, and Pharos). Reference: "A Versatile Automated Sample Changer for Texture Measurements on the High Pressure-preferred Orientation Neutron Diffractometer," *Review of Scientific Instrumentation* **81**, 093302 (2010). The work benefits from the Lujan Neutron Scattering Center at LANSCE, which the DOE Office of Basic Energy Sciences funds.



Schematic sample changer design shown without electronics mounted on top.

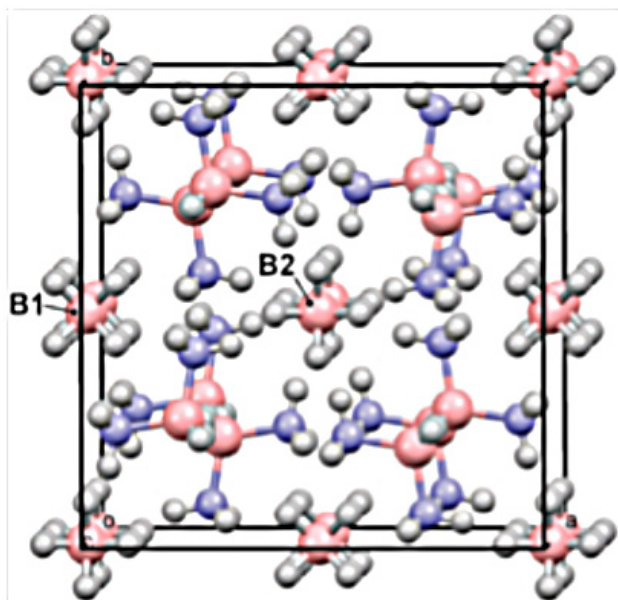
Neutron diffraction sheds light on crystal structure of hydrogen storage material

In the quest for clean energy, solid materials rich in hydrogen, such as ammonia borane, could help solve the gas storage problem for vehicle fuel cells. The crystal structure of an alternative isomeric material, diammoniate of borane (DADB), offers new hope of a stable material that releases hydrogen at a lower temperature (85 °C) rather than the 110 °C of ammonia borane.

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Neutron... Although the stoichiometry of DADB is known, its chemical structure has been the subject of discussion for many years until chemists determined the borohydride formula $[(\text{NH}_3)_2\text{BH}_2]^+[\text{BH}_4]^-$. However, the crystal structure of this important material has not been known until now. Thomas Proffen (LANSCE-LC) and collaborators at the Pacific Northwest National Laboratory have unraveled the crystal structure by adding the data they collected on the Neutron Powder Diffractometer at the Lujan Neutron Scattering Center to the mix of available characterization experiments. The scientists found two crystallographically distinct disordered borohydride $(\text{BH}_4)^-$ sites. Hydrogen release from DADB is similar to that from ammonia borane, but with faster kinetics. Investigators include Mark Bowden, David Heldebrant, Abhi Karkamkar, Gregory Schenter, and Tom Autrey (Pacific Northwest National Laboratory); and Proffen. Reference: "The Diammoniate of Diborane: Crystal Structure and Hydrogen Release," *Chemical Communications* **46**, 8565 (2010). The DOE Office of Basic Energy Sciences supports the Lujan Scattering Center.

Technical contact: Thomas Proffen



Structure of DADB viewed along *c*. The two crystallographically distinct BH_4^- sites are indicated.

Workshop spotlights Lujan Center neutron scattering expertise

Hongwu Xu (Earth System Observations, EES-14), Sven Vogel (LANSCE-LC), and Rudy Wenk (University of California, Berkeley) organized the workshop, "Applications of Neutron Scattering to Materials and Earth Sciences." The University of California, Berkeley sponsored the workshop, which included lectures and tutorials. More than a dozen talks at the event featured the use

of research techniques and instruments at the Laboratory's Lujan Neutron Scattering Center. Los Alamos presenters included Alex Lacerda (LANSCE-DO), Luke Daemen, Katharine Page and Claire White (LANSCE-LC); and Levente Balogh (Structure/Property Relations, MST-8).

The workshop was intended for University of California graduate students, postdoctoral researchers, and other scientists in earth sciences, physics, chemistry, materials science, and engineering interested in applying neutron scattering to studies of synthetic and natural materials. Talks covered the basics of the instruments as well as examples of research by external users of specific applications. The workshop also included data analysis tutorials for information collected from the Lujan Center instruments HIPPO (High Pressure-Preferred Orientation), SMARTS (Spectrometer for Materials Research at Temperature and Stress), NPDF (Neutron Powder Diffractometer), and FDS (Filter Difference Spectrometer). These instruments, among others at LANSCE not covered during this workshop, are used to characterize the atomic structures of materials and the response of the structure to changes in pressure, temperature, and stress.

Approximately 90 interested students and faculty applied to attend the workshop, but space concerns limited participation to 60. The event was the fourth UC-sponsored neutron Lujan workshop and the first held since 2006. Several attendees from non-UC institutions received travel funding from the Consortium for Materials Properties Research in Earth Sciences (COMPRES) network, which fosters high pressure research. The University of California Office of the President also supported travel for UC students and faculty for experiments at LANSCE through a grant awarded to Vogel and Wenk.



Workshop attendees performing data analysis.

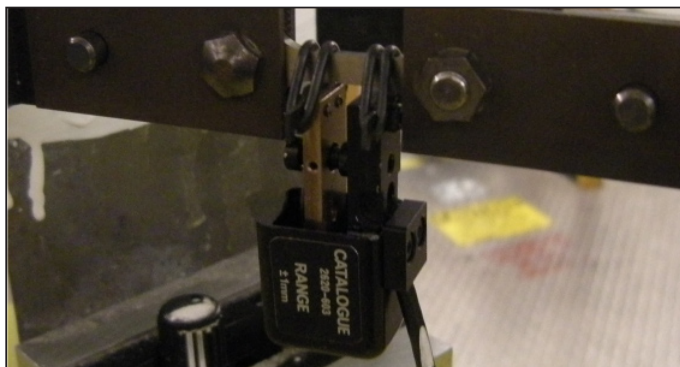
SMARTS examines irradiation-induced evolution of deformation mechanisms

As part of the user program on the SMARTS instrument at the Lujan Neutron Scattering Center, Thomas Sisneros (Structure/Property Relations, MST-8) and Bjorn Clausen (LANSCE-LC) collaborated with the research group of Mark Daymond (Queens University, Kingston, Ontario). The scientists completed in situ neutron diffraction measurements during deformation of radioactive zirconium alloy samples that had been in service in a reactor for approximately 10 years. SMARTS (Spectrometer for Materials Research at Temperature and Stress) employs neutron diffraction techniques to probe metals and structural materials. This experiment is a first step for SMARTS towards experiments on nuclear and radioactive materials. Its success has already motivated future experiments on irradiated steel samples.

Zirconium alloys find application in Canadian nuclear power reactors as cladding for fuel pellets and calandria tubes. The samples emitted 2 REM/hr of combined beta and gamma radiation on contact, necessitating special sample handling procedures that were developed with help from Scott Walker and Mike Duran (Health Physics Operations, RP-1) and Frances Aull (Industrial Safety and Deployed Services, IHS-DS). The scientists completed parallel experiments on matching legacy "pre-installation" material.

Preliminary analysis of the in situ diffraction data shows that the microstructural response of the irradiated and non-irradiated samples was markedly different. This result suggests that a different balance of deformation mechanisms is activated by the irradiation damage in the irradiated sample. Future comparison of the data collected on SMARTS with advanced polycrystalline plasticity models will yield detailed information about the active deformation modes and will be used to improve the existing calculations of in-reactor deformation and component lifetimes. The NSERC (Canadian equivalent of National Science Foundation) as well as the Canadian nuclear power industry funded the work. The DOE Office of Science supports the Lujan Center.

Technical contact: Don Brown



Irradiated zirconium sample mounted in tensile grips on SMARTS.

LANSCE proposal calls

Nuclear Science and ICE House proposal call

LANSCE is accepting proposals for Nuclear Science and ICE House experiments for the run cycle scheduled to begin in June 2011. The deadline for submitting proposals is 6 p.m. (1800) Mountain Standard Time, Wednesday, March 9.

Successful proposals will be scheduled during the period from June through Mid-December 2011 and from January through the end of February 2012.

Proposals must be submitted through the LANSCE Web site. Only proposals submitted online will be accepted. To access the proposal submission site, log onto the LANSCE home page (lansce.lanl.gov). On this page click the link located on the left "WNR" proposal call. This will take you to the online submission system.

First call for Lujan Neutron Scattering Center proposals:

A proposal call is open for beam time at the LANSCE Lujan Neutron Scattering Center for the run cycle scheduled to begin in June 2011. The deadline for submitting the proposals is 6 p.m. (1800) Mountain Standard Time, Wednesday, March 16. Successful proposals will be scheduled during the period June through September 2011. Fast access proposals will be accepted throughout, but require compelling evidence of sufficient scientific urgency to justify scheduling.

Proposals must be submitted through the LANSCE Web site. Only proposals submitted online will be accepted. To access the proposal submission site, log onto the LANSCE home page (lansce.lanl.gov). On this page click the link located on the left "Lujan Center" first call. This will take you to the online submission system.

LANSCE Lujan Center will have a second call for proposals in June and start date notifications will be sent.

Celebrating service

Congratulations to the following AOT and LANSCE Division employees celebrating service anniversaries this month:

Fermin Gonzales, AOT-IC	30 years
Michael Borden, AOT-MDE	25 years
Kenneth Johnson, AOT-ABS	25 years
Joseph Bradley, AOT-RFE	15 years
Alan Hurd, LANSCE-LC	10 years

I'd like to take this opportunity to bring the Division up to speed on the Directorate's progress in implementing the FY11 Environmental Action Plan (EAP) that was developed in support of the Lab's Environmental Management System. Since March 2008, I have served as the Division's representative on the ADEPS team responsible for developing and disseminating the plan. The team currently includes Steve Glick from P Division (the Directorate Point of Contact), Jim Coy from MST, and Cathy Padro from MPA.

I'll start by reminding you of where we were in 2007: the internal EMS audit stated that "...the EMS process in ADEPS lags compared with other directorates...", followed by "Communication of EMS information...was virtually non-existent..." and finishing up with "...15 of 15 workers interviewed were completely unaware of the existence of ADEPS' Environmental Action Plan."

We have gotten substantially better in the past 3 years, with the 2010 findings having a decidedly more positive tone: "ADEPS used a variety of communication tools to deliver EMS info throughout the year;" "Managers were performing environment-focused MOVs ... with several exceeding the number of quarterly environmental MOVs required by the directorate;" and "Strides were made in identifying, consolidating and dispositioning unused and unwanted materials." Melvin Borrego took the lead for LANSCE Division with the disposal of tons of metal waste and in cleaning up the Lujan Center yard. Luke Daemen and Monika Hartl also did a fantastic job in reorganizing the Lujan Center Chemical Laboratory and disposing of legacy samples.

Environmental management will always be an ongoing effort. We humans impact the environment in many ways, and most of the time it is in a negative way. We consume resources, we generate waste, we make mistakes. Our 2011 draft Environmental Action Plan addresses our impact on the environment, and outlines steps we can take to reduce our impact and decrease the potential for and severity of any environmental damage.

Let's look at our objectives, and the specific targets we have developed to meet the objectives. These objectives parallel the LANL institutional objectives, with the targets fine-tuned to fit our Directorate's needs.



2011 Environmental Action Plan for LANSCE

Objective 1: Improve environmental & safety performance via improved integration and communication at the work level. Managers will continue to emphasize environmental aspects during their MOVs, and we will disseminate information on the EAP using posters, group briefings, and e-mails.

Objective 2: Reduce cost & increase efficiency/operating capacity using an approach to P2 (Pollution Prevention). We are working with the Lab's Environmental Team to understand our overall waste generation profile so that we can establish long-term waste-reduction goals. MST will also complete implementation of the MST Chemical Stockroom and MPA will complete the installation of the MPA-11 methanol recirculation and recovery loop to reduce the volume of liquid waste. Both of these projects were competitively selected for Generator Set Aside Funding (GSAF), the Lab program that uses funds collected from waste generators to fund waste-reduction efforts.

Objective 3: Reduce cost and increase efficiency via energy conservation/reductions in fuel, electricity, and H2O consumption. Although this does not affect LANSCE, this one is interesting. Did you know that the MST-OB (03-1415) is one of LANL's High-Efficiency Sustainable Buildings? MST and MPA are going to put together some posters and flyers that inform the occupants and visitors of the energy-efficient aspects of the building.

Objective 4: Implement Lab-wide clean-out activities to disposition unneeded equipment, materials, chemicals, and waste. We continue our annual goal of maintaining a 97% or better chemical inventory via Chemlog database. Since most groups conduct their chemical inventories once a year, it is important to plan to complete the inventory in a timely manner. Plan ahead, and make sure you have a bar-code scanner available. If you need help, please contact me for additional guidance.

Lujan Center plans of further reducing legacy metal, polyethylene shielding, and other items stored in transportainers through disposition.

If anyone at LANSCE has ideas or items they plan on disposing, please let me know so that we may get credit for it! This includes transportainer cleanouts, building cleanouts through salvage, computer disposition, and/or any yard cleanouts.

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Online escorting log

A new online escorting log is now available for use in any Laboratory area with a badge reader, including Property Protection Areas. It is suggested that escorts use the online escorting log or use Access Log Form 1988 to record escort activities for their organizations. To access the online escorting log, visit int.lanl.gov/security/escort/log/.

The online escorting log, which complies with Department of Energy directives, allows:

- only qualified escorts to enter visits on the log;
- escorts to indicate the date and time, technical area, building, and room location for visits; and
- escorts to modify entries in case there is a change in plans.

In addition, entries to the log will trigger an email notification to the host.

Validation

The online escort log is tied to the LANL training and clearance databases. The log will validate escorts' clearance levels and whether the escorts' training records (course number 18366) are current.

Escorts should note that the online escort log cannot validate the background of uncleared visitors (e.g., eligibility to be escorted, citizenship, etc.). Escorts must ensure they verify visitors' escortability.

Escorting reminders

In addition to being qualified, escorts must indicate on the log that they will brief visitors about:

- 1) controlled and prohibited articles prior to entry into the area;
- 2) emergency procedures (e.g., muster areas); and
- 3) any facility-specific requirements.

Important: If the escort log is inaccessible online due to a server or computer problem, the facility owner or responsible line manager for the area may use the Access Log Form 1988.

Resources

- Escorting Help Desk, escortinfo@lanl.gov
- Security Help Desk, 665-2002, security@lanl.gov

For more information, please see the Security Smart at int.lanl.gov/security/documents/security-smart/2010/escortlog1210.pdf

Desk... This June, all divisions in ADEPS will participate in the Lab-wide "Recycle and Reuse Event." I and the other EMS POCs will be collecting any and all items (non bar-coded or classified, of course) that you wish to recycle or get rid of. Details and information on this useful event will be forthcoming; I urge every group to take advantage of this upcoming "spring-cleaning" opportunity.

Objective 5: Reduce long-term impacts, increase operational capacity, and ensure Lab sustainability through an integrated approach to site-wide planning & development.

Ensure future EPS facility environmental sustainability needs are socialized with other lab organizations through active participation in all phases of any new construction projects (such as MaRIE).

Nominate a deserving colleague for a P2 (Pollution Prevention) Award!

Document, Record & Report all significant environmental actions that you take that positively affect the environment. Remember, if it's not recorded, it didn't happen. Please send your environmental action reports (emails are fine) to aull@lanl.gov or to your Group or Center leadership (who will forward it to me), or to the Directorate POC (Steve Glick – sglick@lanl.gov). This will ensure that our Division continues to get the recognition it deserves for our environmental efforts.

Frances Aull, Lujan safety officer

AOT & The Pulse

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To submit news items or for more information,
contact Karen Kippen,
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LALP-11-017

To read past issues see
lansce.lanl.gov/pulse.shtml.

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